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SOME THEORETICAL PROPERTIES OF AN AUGMENTED LAGRANGIAN MERIT FUNCTION

by

Philip B. Gill, Walter Murray, Michael A. Saunders and Margaret H. Wright

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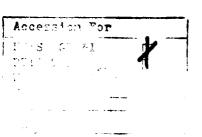
Michael A. Saunders and Margaret H. Wright

Systems Optimization Laboratory

Department of Operations Research

Stanford University

Stanford, California 94305



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ABSTRACT

Sequential quadratic programming (SQP) methods for nonlinearly constrained optimization typically use a merit function to enforce convergence from an arbitrary starting point. We define a smooth augmented Lagrangian merit function in which the Lagrange multiplier estimate is treated as a separate variable, and inequality constraints are handled by means of non-negative slack variables that are included in the linesearch. Global convergence is proved for an SQP algorithm that uses this merit function. We also prove that steps of unity are accepted in a neighborhood of the solution when this merit function is used in a suitable superlinearly convergent algorithm. Finally, a selection of numerical results is presented to illustrate the performance of the associated SQP method.

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1. Sequential Quadratic Programming Methods

Sequential quadratic programming (SQP) methods are widely considered the most effective general techniques for solving optimization problems with nonlinear constraints. (For a survey of results and references on SQP methods, see Powell, 1983.) One of the major issues of interest in recent research on SQP methods has been the choice of merit function—the measure of progress at each iteration. This paper describes some properties of a theoretical SQP algorithm (NPSQP) that uses a smooth augmented Lagrangian merit function. NPSQP is a simplified version of an SQP algorithm that has been implemented as the Fortran code NPSOL (Gill et al., 1985, 1986a, b). (The main simplifications involve the form of the problem and strengthened assumptions.)

For ease of presentation, we assume that all the constraints are nonlinear inequalities. (The theory applies in a straightforward fashion to equality constraints.) The problem to be solved is thus:

NP

minimize
$$F(x)$$

 $x \in \mathbb{R}^n$
subject to $c_i(x) \ge 0$, $i = 1, ..., m$,

where F and $\{c_i\}$ are twice-continuously differentiable. Let g(x) denote the gradient of F(x), and A(x) denote the Jacobian matrix of the constraint vector c(x). The solution of NP will be denoted by x.

We assume that the first-order Kuhn-Tucker conditions hold (with strict complementarity) at x_i^* , i.e., that there exists a Lagrange multiplier vector λ^* such that

$$g(x^*) = A(x^*)^T \lambda^*; \tag{1.1a}$$

$$c(x^*)^T \lambda^* = 0; (1.1b)$$

$$\lambda_i^* > 0 \quad \text{if} \quad c_i(x^*) = 0.$$
 (1.1c)

(For a detailed discussion of optimality conditions, sec, for example, Fiacco and McCormick, 1968, and Powell, 1974.)

At the k-th iteration, the new iterate x_{k+1} is defined as

$$x_{k+1} = x_k + \alpha_k p_k, \tag{1.2}$$

where x_k is the current iterate, p_k is an n-vector (the search direction), and α_k is a non-negative step length $(0 < \alpha_k \le 1)$. For simplicity of notation, we henceforth suppress the subscript k, which will be implicit on unbarred quantities. A barred quantity denotes one evaluated at iteration k+1.

The central feature of an SQP method is that the search direction p in (1.2) is the solution of a quadratic programming subproblem whose objective function approximates the Lagrangian function and whose constraints are linearizations of the nonlinear constraints. The usual definition of the QP subproblem is the following:

minimize
$$g^T p + \frac{1}{2} p^T H p$$
 (1.3a) subject to $Ap \ge -c$, (1.3b)

subject to
$$Ap > -c$$
, (1.3b)

where g, c and A denote the relevant quantities evaluated at x. The matrix H is a symmetric positive-definite quasi-Newton approximation to the Hessian of the Lagrangian function. The Lagrange multiplier vector μ of (1.3) satisfies

$$g + Hp = A^T \mu; \tag{1.4a}$$

$$\mu^T(Ap+c)=0; (1.4b)$$

$$\mu \ge 0. \tag{1.4c}$$

The remainder of this paper is organized as follows. Section 2 gives some background on the role of merit functions within SQP methods, and introduces the augmented Lagrangian merit function used in NPSQP. In Section 3 we state the assumptions about the problem and present the algorithm. Global convergence results are given in Section 4. Section 5 shows that the chosen merit function will not impede superlinear convergence. In Section 6 we present a selection of numerical results to indicate the robustness of the associated SQP method NPSOL.

2. Background on Merit Functions

2.1. Introduction

Many authors have studied the choice of steplength in (1.2). Usually, α is chosen by a linesearch procedure to ensure a "sufficient decrease" (Ortega and Rheinboldt, 1970) in a merit function that combines the objective and constraint functions in some way. A popular merit function for several years (Han, 1976, 1977; Powell, 1977) has been the ℓ_1 penalty function (Pietrzykowski, 1969):

$$P(x,\rho) = F(x) + \rho \sum_{i} \max(0, -c_i(x)). \tag{2.1}$$

This merit function has the property that, for ρ sufficiently large, x^* is an unconstrained minimum of $P(x,\rho)$. In addition, ρ can always be chosen so that the SQP search direction p is a descent direction for $P(x,\rho)$. However, Maratos (1978) observed that requiring a decrease in $P(x,\rho)$ at every iteration could lead to the inhibition of superlinear convergence (see Chamberlain et al., 1982, for a procedure designed to avoid this difficulty). Furthermore, $P(x,\rho)$ is not differentiable at the solution, and linesearch techniques based on smooth polynomial interpolation are thus not applicable.

An alternative merit function that has recently received attention is the augmented Lagrangian function, whose development we now review. If all the constraints of NP are equalities, the associated augmented Lagrangian function is:

$$L(x,\lambda,\rho) \equiv F(x) - \lambda^{T}c(x) + \frac{1}{2}\rho c(x)^{T}c(x), \qquad (2.2)$$

where λ is a multiplier estimate and ρ is a non-negative penalty parameter. Augmented Lagrangian functions were first introduced by Hestenes (1969) and Powell (1969) as a means of

creating a sequence of unconstrained subproblems for the equality-constraint case. A crucial property of (2.2) is that there exists a finite $\hat{\rho}$ such that for all $\rho \geq \hat{\rho}$, x^* is an unconstrained minimum of (2.2) when $\lambda = \lambda^*$ (see, e.g., Fletcher, 1974). The use of (2.2) as a merit function within an SQP method was suggested by Wright (1976) and Schittkowski (1981).

2.2. The Lagrange multiplier estimate

When (2.2) is used as a merit function, it is not obvious—even in the equality-constraint case how the multiplier estimate λ should be defined at each iteration.

Most SQP methods (e.g., Han, 1976; Powell, 1977) define the approximate Hessian of the Lagrangian function using the QP multiplier μ (cf. (1.4)), which can be interpreted as the "latest" (and presumably "best") multiplier estimate, and requires no additional computation. However, using μ as the multiplier estimate in (2.2) has the effect of redefining the merit function at every iteration. Thus, since there is no monotonicity property with respect to a single function, difficulties may arise in proving global convergence of the algorithm.

Powell and Yuan (1984) have recently studied an augmented Lagrangian merit function for the equality-constraint case in which λ in (2.2) is defined as the least-squares multiplier estimate, and hence is treated as a function of x rather than as a separate variable. (An augmented Lagrangian function of this type was first introduced and analyzed as an exact penalty function by Fletcher, 1970.) Powell and Yuan (1984) prove several global and local convergence properties for this merit function.

Other smooth merit functions have been considered by Dixon (1979), DiPillo and Grippo (1979), Bartholomew-Biggs (1983, 1985), and Boggs and Tolle (1984, 1985) (the latter only for the equality-constraint case).

An approach that makes an alternative use of the QP multiplier estimate is to treat the elements of λ as additional variables (rather than to reset λ at every iteration). Thus, a "search direction" ξ is defined for the multiplier estimate, and the linesearch is performed with respect to both x and λ . This idea was suggested by Tapia (1977) in the context of an unconstrained subproblem and by Schittkowski (1981) within an SQP method. This approach will also be taken in NPSQP.

2.3. Treatment of inequality constraints

When defining a merit function for a problem with inequality constraints, it is necessary to identify which constraints are "active". The ℓ_1 merit function (2.1) includes only the violated constraints. The original formulation of an augmented Lagrangian function for inequality constraints is due to Rockafellar (1973):

$$L(x,\lambda,\rho) = F(x) - \lambda^{T}c_{+}(x) + \frac{1}{2}\rho c_{+}(x)^{T}c_{+}(x), \qquad (2.3)$$

where

$$(c_+)_i = \begin{cases} c_i & \text{if } \rho c_i \leq \lambda_i; \\ \lambda_i/\rho & \text{otherwise.} \end{cases}$$

Some global results are given for this merit function in Schittkowski (1981, 1983).

A disadvantage of (2.3) as a merit function is that discontinuities in the first derivative may cause difficulties for linesearch techniques based on polynomial interpolation. Therefore, to retain smoothness during the linesearch even with inequality constraints, we augment the variables (x, λ) by a set of slack variables that are used only in the line search. At the k-th major iteration, a vector triple

$$y = \begin{pmatrix} p \\ \xi \\ q \end{pmatrix} \tag{2.4}$$

is computed that serves as a direction of search for the variables (x, λ, s) . The new values are defined by

$$\begin{pmatrix} \bar{x} \\ \bar{\lambda} \\ \bar{s} \end{pmatrix} = \begin{pmatrix} x \\ \lambda \\ s \end{pmatrix} + \alpha \begin{pmatrix} p \\ \xi \\ q \end{pmatrix}, \tag{2.5}$$

where the vectors p, ξ and q are found from the QP subproblem (1.3), as described below.

In our algorithm (as in Schittkowski, 1981), ξ is defined as

$$\xi \equiv \mu - \lambda, \tag{2.6}$$

so that if $\alpha = 1$, $\bar{\lambda} = \mu$. We take λ_0 as μ_0 (the QP multipliers at x_0), so that $\lambda_1 = \mu_0$ regardless of α_0 .

The definition of s and q can be interpreted in terms of an idea originally given by Rockafellar (1973) in the derivation of (2.3). In our algorithm, the augmented Lagrangian function includes a set of non-negative slack variables:

$$L(x,\lambda,s,\rho) = F(x) - \lambda^{T}(c(x)-s) + \frac{1}{2}\rho(c(x)-s)^{T}(c(x)-s), \quad \text{with} \quad s \geq 0. \tag{2.7}$$

The vector s at the beginning of iteration k is taken as

$$s_{i} = \begin{cases} \max(0, c_{i}) & \text{if } \rho = 0; \\ \max(0, c_{i} - \lambda_{i}/\rho) & \text{otherwise.} \end{cases}$$
 (2.8)

(For given values of x, λ and ρ , the vector s defined by (2.8) yields the value of L minimized with respect to the slack variables alone, subject to the non-negativity restriction $s \geq 0$.) The vector q in (2.5) is then defined by

$$Ap - q = -(c - s), \tag{2.9a}$$

so that

$$Ap+c=s+q. (2.9b)$$

We see from (2.9) that s+q is simply the residual of the inequality constraints from the QP (1.3). Therefore, it follows from (1.3) and (1.4) that

$$s + q \ge 0$$
 and $\mu^{T}(s + q) = 0.$ (2.10)

2.4. Choice of the penalty parameter

Finally, we consider the definition of the penalty parameter in (2.7). Our numerical experiments have suggested strongly that efficient performance is linked to keeping the penalty parameter as small as possible, subject to satisfying the conditions needed for convergence. Hence, our strategy is to maintain a "current" ρ that is increased only when necessary to satisfy a condition that assures global convergence.

Several authors have stated that the need to choose a penalty parameter adds an arbitrary element to an SQP algorithm, or leads to difficulties in implementation. On the contrary, we shall see (Lemma 4.3) that in NPSQP the penalty parameter is based directly on the condition needed for global convergence, and hence should not be considered as arbitrary or heuristic.

3. Statement of Algorithm

We make the following assumptions:

- (i) x and x + p lie in a closed, bounded region Ω of \Re^n for all k;
- (ii) F, $\{c_i\}$, and their first and second derivatives are uniformly bounded in norm in Ω ;
- (iii) H is positive definite, with bounded condition number, and smallest eigenvalue uniformly bounded away from zero, i.e., there exists $\gamma > 0$ such that, for all k,

$$p^T H p \geq \gamma ||p||^2;$$

- (iv) $||\mu||$ is uniformly bounded at every iterate.
- (v) The quadratic program (1.3) always has a solution.

The following notation will be used in the remainder of this section. Given x, λ , s, p, ξ , q and ρ , we let $\phi(\alpha)$ denote $L(x + \alpha p, \lambda + \alpha \xi, s + \alpha q, \rho)$, i.e., the merit function as a function of the steplength. The derivative of ϕ with respect to α will be denoted by ϕ' . Let v denote the "extended" iterate (x, λ, s) , and let y denote the associated search direction (p, ξ, q) . For brevity, we sometimes use the notation " (α) " to denote evaluation at $v + \alpha y$.

The steps of each iteration of algorithm NPSQP are:

- 1. Solve (1.3) for p. If p=0, set $\lambda=\mu$ and terminate. Otherwise, define $\xi=\mu-\lambda$.
- 2. Compute s from (2.8). Find ρ such that $\phi'(0) \leq -\frac{1}{2}p^THp$ (see Lemma 4.3, below).
- 3. Compute the steplength α , as follows. If

$$\phi(1) - \phi(0) < \sigma \phi'(0) \tag{3.1a}$$

and

$$\phi'(1) \le \eta \phi'(0)$$
 or $|\phi'(1)| \le -\eta \phi'(0)$, (3.1b)

where $0 < \sigma \le \eta < \frac{1}{2}$, set $\alpha = 1$. Otherwise, use safeguarded cubic interpolation (see, e.g., Gill and Murray, 1974), to find an $\alpha \in (0,1)$ such that

$$\phi(\alpha) - \phi(0) \le \sigma \alpha \phi'(0) \tag{3.2a}$$

and

$$|\phi'(\alpha)| \le -\eta \phi'(0). \tag{3.2b}$$

- 4. Update H so that (iii) is satisfied (e.g., using a suitably modified BFGS update; see Gill et al., 1986b, for the update used in NPSOL).
- 5. Update x and λ using (2.5).

4. Global Convergence Results

In order to prove global convergence, we first prove a set of lemmas that establish various properties of the algorithm.

Lemma 4.1. Using Algorithm NPSQP, ||p|| = 0 if and only if x is a Kuhn-Tucker point of NP. Furthermore, for x sufficiently close to x^* , the active set of the QP (1.3) is the same as the active set of nonlinear constraints for NP.

Proof. See Robinson (1974).

Lemma 4.2. For all $k \geq 1$,

$$\|\lambda_k\| \leq \max_{1 \leq i \leq k-1} \|\mu_i\|,$$

and hence $\|\lambda_k\|$ is bounded for all k. In addition, $\|\xi_k\|$ is uniformly bounded for all k.

Proof. By definition,

$$\lambda_1 = \mu_0;$$

$$\lambda_{k+1} = \lambda_k + \alpha_k(\mu_k - \lambda_k), \quad k \ge 1.$$
(4.1)

The proof is by induction. The result holds for λ_1 because of assumption (iv) about the boundedness of $||\mu_k||$ for all k. Assume that the lemma holds for λ_k . From (4.1) and norm inequalities, we have

$$||\lambda_{k+1}|| \leq \alpha_k ||\mu_k|| + (1 - \alpha_k) ||\lambda_k||.$$

Since $0 < \alpha \le 1$, applying the inductive hypothesis gives

$$||\lambda_{k+1}|| \leq \max ||\mu_i||, \quad i=1,\ldots,k,$$

which gives the first desired result.

The boundedness of $||\xi_k||$ follows immediately from its definition (2.6), assumption (iv), and the first result of this lemma.

The next lemma establishes the existence of a non-negative penalty parameter such that the projected gradient of the merit function at each iterate satisfies a condition associated with global convergence.

Lemma 4.3. There exists $\hat{\rho} \geq 0$ such that

$$\phi'(0,\rho) \le -\frac{1}{2}p^T H p \tag{4.2}$$

for all $\rho \geq \hat{\rho}$.

Proof. The gradient of L with respect to x, λ and s is given by

$$\nabla L(x,\lambda,s) \equiv \begin{pmatrix} g(x) - A(x)^T \lambda + \rho A(x)^T (c(x) - s) \\ -(c(x) - s) \\ \lambda - \rho(c(x) - s) \end{pmatrix}, \tag{4.3}$$

and it follows that $\phi'(0)$ is given by

$$\phi'(0) = p^{T}g - p^{T}A^{T}\lambda + \rho p^{T}A^{T}(c-s) - (c-s)^{T}\xi + \lambda^{T}q - \rho q^{T}(c-s), \tag{4.4}$$

where g, A, and c are evaluated at x.

Multiplying (1.4a) by p^T gives

$$g^T p = p^T A^T \mu - p^T H p. \tag{4.5}$$

Substituting (2.6), (2.9a) and (4.5) in (4.4), we obtain

$$\phi'(0) = -p^T H p + q^T \mu - 2(c-s)^T \xi - \rho(c-s)^T (c-s). \tag{4.6}$$

Substituting (4.6) in the desired inequality (4.2) and re-arranging, we obtain as the condition to be satisfied

$$q^{T}\mu - 2(c-s)^{T}\xi - \rho(c-s)^{T}(c-s) \le \frac{1}{2}p^{T}Hp.$$
 (4.7)

The complementarity conditions (1.4) and definition (2.9) imply that $q^T \mu \leq 0$. Hence, if $\frac{1}{2}p^T H p > -2(c-s)^T \xi$, then (4.7) holds for all non-negative ρ , and $\hat{\rho}$ may be taken as zero. (Note that this applies when c-s is zero.) The determination of $\hat{\rho}$ is non-trivial only if

$$\frac{1}{2}p^T H p \le -2(c-s)^T \xi. \tag{4.8}$$

Re-arranging (4.7), we see that ρ must satisfy

$$\rho(c-s)^T(c-s) \geq q^T \mu - \frac{1}{2} p^T H p - 2(c-s)^T \xi.$$

A value $\hat{\rho}$ such that (4.8) holds for all $\rho \geq \hat{\rho}$ is given by

$$\hat{\rho} = \frac{2||\xi||}{||c - s||}.\tag{4.9}$$

The penalty parameter ρ in NPSQP is computed by maintaining a "current" value of ρ and modifying it if necessary to satisfy (4.2). Thus, the "new" penalty parameter $\bar{\rho}$ is defined by

$$\bar{\rho} = \begin{cases} \rho & \text{if (4.2) holds;} \\ \max(\hat{\rho}, 2\rho) & \text{otherwise,} \end{cases}$$
 (4.10)

where $\hat{\rho}$ is defined by Lemma 4.3. Note that ρ can become unbounded only if $\hat{\rho}$ is unbounded. Furthermore, (4.10) implies that if ρ is bounded over an infinite sequence of iterations, it must eventually reach a finite value, and will retain that value for all subequent iterations.

We now show that, even if the penalty parameter is unbounded, $\rho ||p||^2$ remains bounded.

Lemma 4.4. If (4.8) holds, then

$$\hat{\rho} \|p\|^2 \le \frac{8\|\xi\|^2}{\gamma},\tag{4.11}$$

where γ is a lower bound on the smallest eigenvalue of H (cf. assumption (iii)).

Proof. From (4.8) and norm inequalities, we have

$$\frac{1}{2}p^T H p \le -2(c-s)^T \xi \le 2||c-s|| ||\xi||, \tag{4.12}$$

which implies

$$||c-s|| \ge \frac{\frac{1}{4}p^T H p}{||\xi||}.$$
 (4.13)

Combining (4.9) and (4.13) and noting that $p^T H p \ge \gamma ||p||^2$, we obtain

$$\hat{\rho} \leq \frac{2||\xi||^2}{\frac{1}{4}p^T H p} \leq \frac{8||\xi||^2}{\gamma ||p||^2}.$$

The desired result follows immediately.

The next two lemmas establish the existence of a step bounded away from zero, independent of k and the size of ρ , for which a sufficient decrease condition is satisfied.

Lemma 4.5. For $0 \le \alpha \le 1$,

$$\phi''(\alpha) = -\phi'(0) + q^{T}\mu + N||p||^{2},$$

where |N| is bounded and independent of k.

Proof. Using (4.3), we have

$$\nabla^2 L = \begin{pmatrix} \nabla^2 F - \sum (\lambda_i + \rho(c_i - s_i)) \nabla^2 c_i + \rho A^T A & -A^T & -\rho A^T \\ -A & 0 & I \\ -\rho A & I & \rho I \end{pmatrix},$$

so that

$$\phi''(\alpha) = y^T \nabla^2 L(v + \alpha y) y = p^T W(\alpha) p - \sum_i \rho \left(c_i(\alpha) - s_i(\alpha) \right) p^T \nabla^2 c_i(\alpha) p + \rho \left(A(\alpha) p - q \right)^T \left(A(\alpha) p - q \right) - 2\xi^T \left(A(\alpha) p - q \right),$$

$$(4.14)$$

where

$$W(\alpha) = \nabla^2 F(\alpha) - \sum_i (\lambda_i + \alpha \xi_i) \nabla^2 c_i(\alpha).$$

We now derive bounds on the first two terms on the right-hand side of (4.14). The first term is bounded in magnitude by a constant multiple of $||p||^2$ because of assumption (ii) and the

boundedness of $\|\lambda\|$ (from Lemma 4.2). For the second term, we expand c_i in a Taylor series about x:

$$c_i(x + \alpha p) = c_i(x) + \alpha a_i(x)^T p + \frac{1}{2} \alpha^2 p^T \nabla^2 c_i(x + \theta_i p) p, \qquad (4.15)$$

where $0 < \theta_i < \alpha$. Since $s_i(\alpha) = s_i + \alpha q_i$, using (2.9a) and multiplying by ρ , we have

$$\rho\left(c_{i}(x+\alpha p)-(s_{i}+\alpha q_{i})\right)=\rho\left(1-\alpha\right)\left(c_{i}(x)-s_{i}\right)+\rho\frac{1}{2}\alpha^{2}p^{T}\nabla^{2}c_{i}(x+\theta_{i}p)p. \tag{4.16}$$

The term $|\rho(c_i(x) - s_i)|$ is uniformly bounded; this follows trivially from the boundedness of $|c_i|$ and $|s_i|$ if ρ is bounded, and from (4.9) if ρ is unbounded. Because $||\nabla^2 c_i||$ is uniformly bounded in the region of interest, a similar argument (using Lemma 4.4 if ρ is unbounded) shows that $|\rho p^T \nabla^2 c_i(x + \theta_i p)p|$ is uniformly bounded. Therefore,

$$|\rho(c_i(\alpha) - s_i(\alpha))| \le J_i, \tag{4.17}$$

where J_i is bounded and independent of the iteration. Using (4.17), we obtain the overall bound

$$\sum |\rho \left(c_i(\alpha) - s_i(\alpha)\right) p^T \nabla^2 c_i(\alpha) p| \le J ||p||^2, \tag{4.18}$$

where J is bounded and independent of the iteration.

Now we examine the third term on the right-hand side of (4.14). Using Taylor series, we have

$$a_i(x + \alpha p)^T p = a_i^T p + \alpha p^T \nabla^2 c_i(\bar{\theta}_i) p, \qquad (4.19)$$

where $0 < \hat{\theta}_i < \alpha$. From (2.9b) and the boundedness of $\|\rho(c-s)\|$ (and Lemma 4.4 if ρ is unbounded), we obtain

$$\rho p^{T} (A(\alpha) - q)^{T} (A(\alpha)p - q) = \rho (c - s)^{T} (c - s) + L||p||^{2}, \tag{4.20}$$

where |L| is bounded and independent of the iteration.

Using (4.19) and the boundedness of $\|\xi\|$, the final term on the right-hand side of (4.14) can be written as

$$-2\xi^{T}(A(\alpha)p-q)=2\xi^{T}(c(x)-s)+M||p||^{2}, \qquad (4.21)$$

where |M| is bounded and independent of the iteration.

Combining (1.20) and (4.21), the last two terms on the right-hand side of (4.14) become

$$\rho (A(\alpha)p - q)^{T} (A(\alpha)p - q) - 2\xi^{T} (A(\alpha)p - q) = \rho (c - s)^{T} (c - s) + 2\xi^{T} (c - s) + \bar{M} ||p||^{2}$$
$$= -\phi'(0) + q^{T} \mu + \bar{M} ||p||^{2},$$

where $|\bar{M}|$ is bounded and independent of the iteration (using (4.6) and noting that the largest eigenvalue of H is bounded).

Combining all these bounds gives the required result.

Lemma 4.6. The linesearch in Step 3 of the algorithm defines a step length α (0 < $\alpha \le 1$) such that

$$\phi(\alpha) - \phi(0) \le \sigma \alpha \phi'(0), \tag{4.22}$$

and $\alpha \geq \bar{\alpha}$, where $0 < \sigma < 1$, and $\bar{\alpha} > 0$ is bounded away from zero and independent of the iteration.

Proof. If both conditions (3.1) are satisfied, then $\alpha = 1$ and (4.22) holds with α trivially bounded away from zero.

Assume that (3.1) does not hold (i.e., α is computed by safeguarded cubic interpolation). The existence of a step length α that satisfies conditions (3.2) is guaranteed from standard analysis (see, for example, Moré and Sorensen, 1984). We need to show that α is uniformly bounded away from zero. There are two cases to consider.

First, assume that (3.1a) does not hold, i.e., $\phi(1) - \phi(0) > \sigma \phi'(0)$. Since $\phi'(0) < 0$, this implies the existence of at least one positive zero of the function

$$\psi(\alpha) = \phi(\alpha) - \phi(0) - \sigma\alpha\phi'(0).$$

Let α^* denote the smallest such zero. Since ψ vanishes at zero and α^* , and $\psi'(0) < 0$, the mean-value theorem implies the existence of a point $\hat{\alpha}$ $(0 < \hat{\alpha} < \alpha^*)$ such that $\psi'(\hat{\alpha}) = 0$, i.e., for which

$$\phi'(\hat{\alpha}) = \sigma \phi'(0).$$

Because $\sigma \leq \eta$, it follows that

$$\phi'(\hat{\alpha}) - \eta \phi'(0) = (\sigma - \eta)\phi'(0) \geq 0.$$

Therefore, since the function $\phi'(\alpha) - \eta \phi'(0)$ is negative at $\alpha = 0$, and non-negative at $\hat{\alpha}$, the mean-value theorem again implies the existence of a smallest value $\bar{\alpha}$ $(0 < \bar{\alpha} \le \hat{\alpha})$ such that

$$\phi'(\bar{\alpha}) = \eta \phi'(0). \tag{4.23}$$

The point $\bar{\alpha}$ is the required lower bound on the step length because (4.23) implies that (3.2b) will not be satisfied for any $\alpha \in [0, \bar{\alpha})$.

Expanding ϕ' in a Taylor series gives

$$\phi'(\bar{\alpha}) = \phi'(0) + \bar{\alpha}\phi''(\theta),$$

where $0 < \theta < \tilde{\alpha}$. Therefore, using (4.23) and noting that $\eta < 1$ and $\phi'(0) < 0$, we obtain

$$\bar{\alpha} = \frac{\phi'(\bar{\alpha}) - \phi'(0)}{\phi''(\theta)} = (1 - \eta) \frac{|\phi'(0)|}{\phi''(\theta)}.$$
 (4.24)

(Since $\bar{\alpha} > 0$, θ must be such that $\phi''(\theta) > 0$.) We seek a lower bound on $\bar{\alpha}$, and hence an upper bound on the denominator of (4.24). We know from Lemma 4.5 that

$$\phi''(\theta) = -\phi'(0) + q^{T} \mu + N ||p||^{2},$$

and from (2.10) that $q^T \mu \leq 0$. Therefore,

$$\phi''(\theta) \le |\phi'(0)| + |N| ||p||^2,$$

and hence

$$\bar{\alpha} \geq \frac{(1-\eta)|\phi'(0)|}{|\phi'(0)| + |N|||p||^2}.$$

Dividing by $|\phi'(0)|$ gives

$$\tilde{\alpha} \ge \frac{(1-\eta)}{1+\frac{|N|||p||^2}{|\phi'(0)|}}.$$
(4.25)

Since the algorithm guarantees that $\phi'(0) \leq -\frac{1}{2}p^THp$, it follows that

$$|\phi'(0)| \ge \frac{1}{2} p^T H p \ge \frac{1}{2} \gamma ||p||^2, \tag{4.26}$$

where γ is bounded below. Thus, the denominator of (4.25) may be bounded above as follows:

$$1 + \frac{|N|||p||^2}{|\phi'(0)|} \le 1 + \frac{|N|||p||^2}{\frac{1}{2}\gamma||p||^2} = 1 + \frac{2|N|}{\gamma}.$$

A uniform lower bound on $\bar{\alpha}$ is accordingly given by

$$\bar{\alpha} \ge \frac{\gamma(1-\eta)}{\gamma+2|N|}.\tag{4.27}$$

In the second case, we assume that (3.1a) is satisfied, but (3.1b) is not. In this case, it must hold that $\phi'(1) \geq 0$, and hence $\phi'(\alpha)$ must have at least one zero in (0,1]. If $\bar{\alpha}$ denotes the smallest of these zeros, $\bar{\alpha}$ satisfies (4.23), and (4.27) is again a uniform lower bound on the step length.

The proof of a global convergence theorem is now straightforward.

Theorem 4.1. Under assumptions (i)-(v), the algorithm defined by (1.2), (1.3), (4.2), and (4.22) has the property that

$$\lim_{k\to\infty}||p_k||=0. (4.28)$$

Proof. If $||p_k|| = 0$ for any finite k, the algorithm terminates and the theorem is true. Hence we assume that $||p_k|| \neq 0$ for any k. There are two cases to consider.

First, assume that ρ is unbounded. In this case, the discussion following Lemma 4.3 shows that $\hat{\rho}$ must be unbounded, and hence we know from Lemma 4.4 that

$$||p||^2 \le \frac{8||\xi||}{\gamma \hat{\rho}}.\tag{4.29}$$

Since $\|\xi\|$ is bounded, the desired result follows immediately.

Second, assume that ρ is bounded. The discussion following Lemma 4.3 shows that in this case ρ must eventually become fixed at a given finite value, i.e., there exists a value $\tilde{\rho}$ and an iteration index \tilde{K} such that $\rho = \tilde{\rho}$ for all $k \geq \tilde{K}$. We consider henceforth only such values of k.

The proof is by contradiction. We assume that there exists $\epsilon > 0$ and $K \ge \tilde{K}$ such that $||p_k|| \ge \epsilon$ for $k \ge K$. Every subsequent iteration must therefore yield a strict decrease in the merit function (2.7) with $\rho = \tilde{\rho}$, because, using (4.22),

$$\phi(\alpha) - \phi(0) \le \eta \alpha \phi'(0) \le \frac{1}{2} \eta \ddot{\alpha} \gamma \epsilon^2 < 0.$$

The two final inequalities are derived from Lemma 4.6, since $\alpha \geq \bar{\alpha}$, which is uniformly bounded away from zero. The adjustment of the slack variables s in Step 2 of the algorithm can only lead to a further reduction in the merit function. Therefore, since the merit function with $\rho = \tilde{\rho}$ decreases by at least a fixed quantity at every iteration, it must be unbounded below. But this is impossible, from assumptions (i)-(ii) and Lemma 4.2. Therefore, (4.28) must hold.

Corollary 4.1.

$$\lim_{k\to\infty}||x_k-x^*||=0.$$

Proof. The result follows immediately from Theorem 4.1 and Lemma 4.1.

The second theorem shows that Algorithm NPSQP also exhibits convergence of the multiplier estimate λ .

Theorem 4.2. If $\hat{A}(x^*)$, the Jacobian matrix of the constraints active at x^* , has full rank, then

$$\lim_{k\to\infty}||\lambda_k-\lambda^*||=0.$$

Proof. If $||p_k|| = 0$, then $\mu_k = \lambda^*$ (using (1.1) and (1.4)); in Step 1 of Algorithm NPSQP, λ_{k+1} is set to λ^* , and the algorithm terminates. Thus, the theorem is true if $p_k = 0$ for any k. We therefore assume that $||p_k|| \neq 0$ for any k.

The definition (4.1) gives

$$\lambda_{k+1} = \sum_{i=0}^{k} \gamma_{ik} \mu_i, \tag{4.30}$$

where

$$\gamma_{kk} = \alpha'_k$$
 and $\gamma_{ik} = \alpha'_i \prod_{j=i+1}^k (1 - \alpha'_j), \quad i < k,$ (4.31)

with $\alpha_0' = 1$ and $\alpha_i' = \alpha_i$, $i \ge 1$. (This convention is used because of the special initial condition that $\lambda_0 = \mu_0$.) From Lemma 4.6 and (4.31), we observe that

$$0 < \tilde{\alpha} \le \alpha_i' \le 1$$
 for all i , (4.32a)

$$\sum_{i=0}^k \gamma_{ik} = 1 \tag{4.32b}$$

and

$$\gamma_{ik} \le (1 - \bar{\alpha})^{k-i}, \quad i < k. \tag{4.32c}$$

Since we know from Theorem 4.1 that $x_k \to x^*$, the iterates will eventually reach a neighborhood of x^* in which the QP subproblem identifies the correct active set (Lemma 4.1) and $\hat{A}(x_k)$ has full rank. Assume that these properties hold for $k \geq K_1$. From the definition (1.4) of μ , assumptions (ii)-(iii), and the existence of a lower bound on the smallest singular value of \hat{A} , we have for $k \geq K_1$ that there exists a bounded scalar M such that

$$\mu_k = \lambda^* + M_k d_k t_k, \tag{4.33}$$

with $|M_k| \leq M$, $d_k = \max(||p_k||, ||x^* - x_k||)$ and $||t_k|| = 1$. Given any $\epsilon > 0$, Theorem 4.1 and Corollary 4.1 also imply that K_1 can be chosen so that, for $k \geq K_1$,

$$|M_k d_k| \le \frac{1}{2}\epsilon. \tag{4.34}$$

We can also define an iteration index K_2 with the following property:

$$(1-\bar{\alpha})^k \leq \frac{\epsilon}{2(k+1)(1+\bar{\mu}+||\lambda^k||)} \tag{4.35}$$

for $k \ge K_2 + 1$, where $\bar{\mu}$ is an upper bound on $\|\mu\|$ for all k. Let $K = \max(K_1, K_2)$. Then, from (4.30) and (4.33), we have for $k \ge 2K$,

$$\lambda_{k+1} = \sum_{i=0}^{K} \gamma_{ik} \mu_i + \sum_{i=K+1}^{k} \gamma_{ik} (\lambda^* + M_i d_i t_i).$$

Hence it follows from (4.32b) that:

$$\lambda_{k+1} - \lambda^* = \sum_{i=0}^K \gamma_{ik} (\mu_i - \lambda^*) + \sum_{i=K+1}^k \gamma_{ik} M_i d_i t_i.$$

From the bounds on $\|\mu_i\|$ and $\|t_i\|$ we then obtain

$$\|\lambda_{k+1} - \lambda^*\| \le (\bar{\mu} + \|\lambda^*\|) \sum_{i=0}^K \gamma_{ik} + \sum_{i=K+1}^k \gamma_{ik} |M_i d_i|. \tag{4.36}$$

Since $k \geq 2K$, it follows from (4.32a) and (4.32c) that

$$\sum_{i=0}^{K} \gamma_{ik} \leq \sum_{i=0}^{K} (1-\alpha)^{k+i} \leq \sum_{i=0}^{K} (1-\alpha)^{2K-i} \leq (K+1)(1-\alpha)^{K}.$$

Using (4.35), we thus obtain the following bound for the first term on the right-hand side of (4.36):

$$(\bar{\mu} + ||\lambda^*||) \sum_{i=0}^K \gamma_{ik} \leq \frac{1}{2} \epsilon. \tag{4.37}$$

To bound the second term in (4.36), we use (4.32b) and (4.34):

$$\sum_{i=K+1}^{k} \gamma_{ik} |M_i d_i| \leq \frac{1}{2} \epsilon \sum_{i=K+1}^{k} \gamma_{ik} \leq \frac{1}{2} \epsilon. \tag{4.38}$$

Combining (4.36)-(4.38), we obtain the following result: given any $\epsilon > 0$, we can find K such that

$$\|\lambda_k - \lambda^*\| \le \epsilon \quad \text{for} \quad k \ge 2K + 1,$$

which implies that

$$\lim_{k\to\infty}\|\lambda_k-\lambda^*\|=0.$$

5. Use within a Superlinearly Convergent Algorithm

As mentioned in Section 2.1, a point of interest is whether superlinear convergence may be impeded by the requirement of a sufficient decrease in the merit function at every iteration. In this section we show that a unit step ($\alpha = 1$) will satisfy conditions (3.1) when the iterates are sufficiently close to the solution and x and λ are converging superlinearly at the same rate. For further discussion of superlinear convergence, see Dennis and Moré (1977) and Boggs, Tolle and Wang (1982).

In addition to the conditions assumed in the previous section, we assume that for all sufficiently large k:

$$x_k + p_k - x^* = o(||x_k - x^*||),$$
 (5.1a)

$$\lambda_k + \xi_k - \lambda^* = o(||\lambda_k - \lambda^*||), \tag{5.16}$$

$$\frac{||p_k||}{||\xi_k||} > M > 0, (5.1c)$$

where M is independent of K. Note that (5.1) implies

$$||p_k|| \sim ||x_k - x^*||$$
 and $||\xi_k|| \sim ||\lambda_k - \lambda^*||$, (5.2)

where " \sim " means that the two quantities are of similar order. (See also Dennis and Moré, 1977.) First we show that these assumptions imply that the penalty parameter ρ in the merit function (2.7) must remain bounded for all k. **Lemma 5.1.** Under assumptions (i) (v) of Section 3, and conditions (5.1), there exists a finite $\bar{\rho}$ such that for all k,

$$\rho \le \ddot{\rho}.\tag{5.3}$$

Proof. Recall from the proof of Lemma 4.3 that ρ can become unbounded only if (4.8) holds and $\hat{\rho}$ as defined by (4.9) becomes unbounded. Condition (4.8) states that $-2(c-s)^T\xi \geq \frac{1}{2}p^THp$. Using assumption (iii) and norm inequalities, (4.8) thus implies

$$||c-s|| \geq \frac{\frac{1}{4}\gamma ||p||^2}{||\xi||}.$$

Hence, from (5.1c), we obtain

$$\frac{||c-s||}{||\xi||} \ge \frac{\frac{1}{4}\gamma||p||^2}{||\xi||^2} = \bar{M} > 0.$$

Consequently, from Lemma 4.4,

$$\hat{
ho}<rac{2}{ar{M}},$$

and remains bounded. This proves the lemma.

The next two lemmas show that conditions (3.1) are eventually satisfied for all k sufficiently large.

Lemma 5.2. Under assumptions (i)-(v) of Section 3 and conditions (5.1), the sufficient decrease condition (3.1a) holds for sufficiently large k, i.e.,

$$\phi(1)-\phi(0)\leq\sigma\phi'(0),$$

where $0 < \sigma < \frac{1}{2}$.

Proof. As in Powell and Yuan (1984), observe that the continuity of second derivatives gives the following relationships:

$$F(x+p) = F(x) + \frac{1}{2} (g(x) + g(x+p))^{T} p + o(||p||^{2}),$$

$$c(x+p) = c(x) + \frac{1}{2} (A(x) + A(x+p)) p + o(||p||^{2}).$$

Conditions (5.1) and (5.2) then imply:

$$F(x+p) = F(x) + \frac{1}{2} (g(x) + g(x^*))^T p + o(||p||^2), \tag{5.4a}$$

$$c(x+p) = c(x) + \frac{1}{2} (A(x) + A(x^*)) p + o(||p||^2).$$
 (5.4b)

We shall henceforth use g to denote g(x) and g^* to denote $g(x^*)$, and similarly for F, c and A.

By definition,

$$\phi(0) = F - \lambda^T (c - s) + \frac{1}{2} \beta(c - s)^T (c + s),$$
 (5.5a)

$$\phi(1) = F(x+p) - \mu^T(c(x+p) - c + Ap)$$

$$+\frac{1}{2}\rho(c(x+p)-c-Ap)^{T}(c(x+p)-c-Ap).$$
 (5.5b)

Using Taylor series, we have

$$c(r+p) = c + Ap + O(|p||^2).$$
 (5.6)

Substituting from (5.4) and (5.6) into (5.5b), we obtain

$$\phi(1) = F + \frac{1}{2}(g + g^*)^T p + \frac{1}{2}\mu^T (A - A^*) p + o(\|p\|^2).$$
 (5.7)

Combining (5.5a) and (5.7) gives

$$\phi(1) = \phi(0) = \frac{1}{2}p^{T}g + \frac{1}{2}p^{T}g^{*} + \frac{1}{2}\mu^{T}Ap + \frac{1}{2}\mu^{T}A^{*}p + \lambda^{T}(c - s) - \frac{1}{2}\rho(c - s)^{T}(c - s) + o(||p||^{2}).$$
(5.8)

Using (2.6), (2.9) and (4.4), we obtain the following expression:

$$\phi'(0) = p^{T}g + 2\lambda^{T}(c - s) - \rho(c - s)^{T}(c - s) + \mu^{T}Ap - \mu^{T}q.$$
 (5.9)

Substituting (5.9) into (5.8), we have

$$\phi(1) - \phi(0) = \frac{1}{2}\phi'(0) + \frac{1}{2}\mu^{T}q + \frac{1}{2}p^{T}(g^{*} - A^{*T}\mu) + o(||p||^{2}).$$
 (5.10)

It follows from (5.1b) (5.1c) that the expression $g^* = A^* \frac{r}{\mu}$ is $o(||p_0^{\mu}|)$, which gives

$$egin{aligned} \phi(1) &= \phi(0) = rac{1}{2} \phi'(0) + rac{1}{2} \mu^T q + o(\|oldsymbol{p}\|^2) \ &+ rac{1}{2} \phi'(0) + o(^{\alpha} p)^2), \end{aligned}$$

and hence

$$\phi(1) = \phi(0) + \sigma \phi'(0) < (\frac{1}{2} + \sigma)\phi'(0) + o(||p||^2).$$
 (5.11)

Since $\sigma < \frac{1}{2}$ and $\phi'(0)$ satisfies (4.2), (5.11) implies that (3.1a) holds for sufficiently large k.

Lemma 5.3. Under assumptions (i) (v) and conditions (5.1), the second linesearch condition (3.1b) holds for sufficiently large k, i.e.,

$$\phi'(1) \leq \eta \phi'(0) \quad \text{or} \quad |\phi'(1)| \leq \eta_i \phi'(0)|,$$

where $\eta < \frac{1}{2}$.

Proof. In this proof, we use the notation q(1) to denote q(x+p), and similarly for c and A. Using (4.3), $\phi'(1)$ is given by

$$\phi'(1) = p^{T}g(1) - p^{T}A(1)\mu + \rho p^{T}(c(1) - c - Ap) + q^{T}\mu - \rho q^{T}(c(1) + c - Ap).$$
(5.12)

6. Numerical Results

From conditions (5.2) (5.3), we have

$$g(1) = g^* + o(||p||^2), \quad A(1) = A^* + o(||p||^2) \quad \text{and} \quad \mu = \lambda^* + o(||p||).$$
 (5.13)

Substituting from (5.6) and (5.13) into (5.12) then gives:

$$\phi'(1) = p^T g^* - p^T A^* \mu + q^T \mu - \rho(c - s)^T (c(1) - c - Ap) + o(||p||^2).$$
 (5.14)

Consider now the vectors (c-s), q and μ . From (2.8) and (5.2), ||c-s|| = O(||p||). From Lemma 4.1, we know that the QP subproblem (1.3) will eventually predict the correct active set, and hence that $\mu_i = 0$ if $c_i(x^*) > 0$. For an active constraint c_i , it follows from (2.8) that s_i will eventually be set to zero at the beginning of every iteration if $\rho > 0$, and hence q_i must also be zero. If $\rho = 0$ and c_i is an active constraint, then $|q_i| = o(||p||^2)$. Therefore, in either case we have that

$$|q^T \mu| = o(||p||^2)$$
 and $|\rho(c-s)^T (c(1) - c - Ap)| = o(||p||^2).$ (5.15)

Recalling that $||g^* - A^{*T}\mu|| = o(||p||)$ and using (5.15) in (5.14), we obtain

$$\phi'(1) = o(||p||^2). (5.16)$$

Since $|\phi'(0)| \ge \frac{1}{2}\gamma ||p||^2$, (5.16) implies that (3.1b) will eventually be satisfied at every iteration.

6. Numerical Results

In order to indicate the reliability and efficiency of a practical SQP algorithm based on the merit function (2.7), we present a selection of numerical results obtained from the Fortran code NPSOL (Gill et al., 1986a, b). Table 1 contains the results of solving a subset of problems 70-119 from Hock and Schittkowski (1981). (We have omitted problems that are non-differentiable or that contain only linear constraints. Since NPSOL treats linear constraints separately, they do not affect the merit function.)

The problems were run on an IBM 3081K, in double precision (i.e., machine precision ϵ_M is approximately 2.22×10^{-16}). The default parameters for NPSOL were used in all cases (for details, see Gill et al., 1986a). In particular, the default value for ftol, the final accuracy requested in F, is 5.4×10^{-12} , and ctol, the feasibility tolerance, is $\sqrt{\epsilon_M}$. Analytic gradients were provided for all functions, and a gradient linesearch was used.

For successful termination of NPSOL, the iterative sequence of x-values must have converged and the final point must satisfy the first-order Kuhn-Tucker conditions (cf. (1.1)). The sequence of iterates is considered to have converged at x if

$$\alpha ||p|| \leq \sqrt{ftol} \left(1 + ||x||\right),\tag{6.1}$$

where p is the search direction and α the step length from (1.2). The iterate x is considered to satisfy the first-order conditions for a minimum if the following conditions hold: the inactive

constraints are satisfied to within ctol, the magnitude of each active constraint residual is less than ctol, and

$$||Z(x)^T g(x)|| \le \sqrt{ftol} \left(1 + \max(1 + |F(x)|, ||g(x)||)\right),$$
 (6.2)

where Z(x) is an orthogonal basis for the null space of the gradients of the active constraints. (Thus, $Z(x)^T g(x)$ is the usual projected gradient.)

Table 1 gives the following information: the problem number in Hock and Schittkowski; the number of variables (n); the number of simple bounds (m_B) ; the number of general linear constraints (m_L) ; the number of nonlinear constraints (m_N) ; the number of iterations; and the number of function evaluations. (Each constraint is assumed to include a lower and an upper bound.)

Table 1

Problem	n	m_B	m_L	m_N	Iterations	Evaluations
70	4	4	0	1	35	38
71	4	4	0	2	5	6
72	4	4	0	2	6	7
73	4	4	2	1	3	4
74	4	4	2	3	9	10
75	4	4	2	3	7	8
77	5	0	0	2	14	20
78	5	0	0	3	8	10
79	5	0	0	3	9	12
80	5	5	0	3	8	10
81	5	5	0	3	9	10
83	5	5	0	3	4	6
84	5	5	0	3	5	6
85	5	5	0	38	45	68
93	6	6	0	2	11	14
95	6	6	0	4	1	2
96	6	6	0	4	1	2
97	6	6	0	4	3	6
98	6	6	0	4	3	6
99	7	7	0	2	19	34
100	7	0	0	4	15	34
101	7	7	0	5	33	85
102	7	7	0	5	29	69
103	7	7	0	5	25	60
104	8	8	0	5	17	19
106	8	8	3	3	43	47
107	9	7	0	6	11	18
108	9	1	0	13	15	19
109	9	9	1	8	18	19
111	10	10	0	3	59	62
113	10	0	3	5	14	19
114	10	10	5	6	51	81
116	13	13	5	10	54	78
117	15	15	0	5	19	20

NPSOL terminated successfully on all the problems except the badly scaled problem 85, for which (6.1) could not be satisfied. However, the optimality conditions were satisfied at the final iterate, which gave an improved objective value compared to that in Hock and Schittkowski (1981).

7. References

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SOL 86-6: "Some Theoretical Properties of an Augmented Lagrangian Merit Function," Philip E. Gill, Walter Murray, Michael A. Saunders & Margaret H. Wright

Sequential quadratic programming (SQP) methods for nonlinearly constrained optimization typically use a <u>merit function</u> to enforce convergence from an arbitrary starting point. We define a <u>smooth</u> augmented Lagrangian merit function in which the Lagrange multiplier estimate is treated as a separate variable, and inequality constraints are handled by means of non-negative slack variables that are included in the linesearch. Global convergence is proved for an SQP algorithm that uses his merit function. We also prove that steps of unity are accepted in a neighborhood of the solution when this merit function is used in a suitable superlinearly convergent algorithm. Finally, a selection of numerical results is presented to illustrate the performance of the associated SQP method.

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